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\textbf{ABSTRACT:}

A benefit of hydrogen as an energy carrier is that it can be produced from a diverse set of energy resources by means of a variety of process technologies. Energy resources include fossil, renewable, and nuclear energy; while process technologies include thermochemical, electrochemical, photolytic, and biological processes. We used the analytical tools H2A and GREET to evaluate several hydrogen production pathways in terms of energy efficiency, greenhouse gas emissions, and cost. We evaluated central and distributed production facilities, the distinction being the quantity of hydrogen produced (in kilograms or gasoline gallon equivalents (gge) of hydrogen per day). For relatively immature production pathways, we assessed the state of technology. Critical technical barriers that must be overcome to realize the potential of these technologies are discussed.

\textbf{KEYWORDS:} production, delivery, emissions, costs

\section*{Introduction}

The U.S. Department of Energy (DOE) envisions a future energy economy for the United States that features two predominant energy carriers: hydrogen and electricity. Hydrogen, in particular, is attractive because it can be produced from a diverse set of energy resources using several process technologies and can be used in advanced vehicle technologies such as fuel-cell vehicles. Possible resources for producing hydrogen include fossil, renewable, and nuclear energy. Technologies for producing hydrogen include thermochemical, electrochemical, photolytic, and biological processes.

Today hydrogen is produced principally from natural gas. As part of its goal to increase national energy security, DOE’s long-term strategy is to produce hydrogen from various renewable energy sources (including solar energy, wind, biomass, hydropower, and geothermal energy), nuclear energy, and domestic coal (with sequestration of CO\textsubscript{2}).

Comparing the feasibility of various options for hydrogen production requires analysis tools that can be used in a transparent, consistent manner. The U.S. DOE is working through its national laboratories and industry contractors to develop analysis tools that will allow researchers and policy makers to examine various energy source and process technology scenarios.

\section*{Methods}

Researchers in the U.S. DOE Hydrogen Program used the analytical tools H2A\textsuperscript{1} and GREET\textsuperscript{2} to evaluate several hydrogen production pathways in terms of energy efficiency, emission of greenhouse gases, and cost\textsuperscript{3}. Central and distributed production facilities were evaluated. For relatively immature production pathways, we assessed the state of technology using available information.

\textbf{H2A}

DOE’s Office of Energy Efficiency and Renewable Energy (EERE) developed the Hydrogen Analysis (H2A) suite of models to improve the transparency and consistency of hydrogen pathway analysis. The H2A production models assess the cost of producing hydrogen at central and forecourt (station) facilities. This interactive tool allows the user to define several process characteristics, including process design, facility capacity, capacity factor, energy efficiency, and feedstock requirements. While the tool includes H2A reference values for several financial parameters, the user is also given the opportunity to vary parameters such as internal rate of return (IRR), plant life, feedstock costs, and tax rate to examine the technology using an alternative set of assumptions. The calculation part of the tool uses a standard discounted cash flow rate
of return analysis methodology to determine the required hydrogen selling price necessary to obtain the desired IRR.

The H2A model suite is spreadsheet-based and draws the best available information about capital and operating costs, energy and feedstock consumption, and environmental emissions from public literature. In most cases, information is supported by a process simulation model such as ASPEN Plus®. The H2A models are available to the public at http://www.hydrogen.energy.gov/h2a_analysis.html.

Hydrogen costs presented in this paper were determined using the H2A production model, and were modified to reflect the U.S. DOE’s Hydrogen, Fuel Cells, and Infrastructure Technologies Program cost goals as of November 2005. These costs reflect the minimum hydrogen selling price required to obtain a 10% IRR. Efficiency results are presented in terms of the lower heating value of hydrogen. Costs for fossil fuel feedstocks are based upon price projections from the U.S. DOE’s Energy Information Agency’s Annual Energy Outlook 2005 High A Case. The result from the model is the necessary selling price of hydrogen required to obtain a 10% IRR after taxes. It is important to understand that this is neither a predicted market price nor a reflection of the current price of hydrogen from existing facilities.

**GREET**

The GREET (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) model is used to evaluate energy and emission impacts of advanced vehicle technologies and new transportation fuels wells to wheels (or the fuel cycle). This model allows researchers and analysts to evaluate various vehicle and fuel combinations on a full fuel-cycle basis. As of now, there are more 2,800 registered GREET users worldwide.

GREET was developed as a multidimensional spreadsheet model in Microsoft Excel and uses a graphic user interface (GUI) program. This model is available for public use through http://www.transportation.anl.gov/software/GREET/.

For a given vehicle and fuel system, GREET separately calculates the following:

- Consumption of total energy (energy in non-renewable and renewable sources), fossil fuels (petroleum, natural gas, and coal), and petroleum,
- Emissions of CO₂-equivalent greenhouse gases - primarily carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O),
- Emissions of five criteria pollutants: volatile organic compounds (VOCs), carbon monoxide (CO), nitrogen oxides (NOₓ), particulate matter with size smaller than 10 micron (PM₁₀), and sulfur oxides (SOₓ). Emissions of these pollutants are further separated into total emissions and urban emissions.

For this study, we estimated well-to-wheels energy and petroleum use and greenhouse gas emissions using the GREET model, Version 1.7, the most recent version of the GREET model. These values represent primary fuel production, electricity production, and hydrogen production, compression, and dispensing. Equipment manufacture is not included.

**Results**

Results of estimated energy use per vehicle mile traveled on a “well-to-wheels” basis are shown in Figure 1 for several cases. The bar on the left for each case is the total energy use (petroleum plus other fossil energy plus renewable energy). The other bar for each case is petroleum energy use. The two gasoline-fueled vehicle cases on the left have energy use principally from petroleum. For fuel cell vehicles, the petroleum energy use in each case is shown multiplied by a factor of ten to make the information visible on the chart.
Figures 2-4 show estimated emissions of greenhouse gases per vehicle mile traveled, cost of hydrogen, and pathway energy efficiency for the same cases.
Figure 3. Necessary Selling Price of Delivered Hydrogen

Figure 4. Hydrogen Pathway Energy Efficiency
Natural Gas
Hydrogen as an energy carrier may be introduced into the marketplace through distributed reforming of natural gas. Our analysis for this case included a steam reformer, water-gas shift reactors, pressure swing adsorption unit, and compression, storage and dispensing equipment. The entire system was sized to provide about 1,500 gasoline-gallon equivalents (gge) of hydrogen assuming a 70% operating capacity factor. (A gasoline-gallon equivalent of hydrogen is approximately equal to the energy content in a kilogram of hydrogen.)

Two cases are shown for distributed hydrogen production via steam methane reforming: current 2005 technology and a future case of 2015 technology. The 2015 case is based upon the U.S. DOE’s hydrogen program cost goal. The total estimated energy consumption for the 2005 and 2015 cases is 3,700 and 2,800 British thermal units (Btu) per mile of automobile travel (1 Btu/mile equals 0.658 kiloJoules/kilometer), respectively. These figures compare to 5,900 and 4,200 Btu/mile for current gasoline internal combustion engine automobiles and gasoline electric hybrid automobiles, respectively.

Greenhouse gas emissions for the distributed SMR case are less than for the gasoline internal combustion engine and hybrid vehicle cases. The required selling price of hydrogen to obtain a 10% IRR is $3.10 and $2.00/gge for the current and future cases, respectively. Pathway energy efficiencies are 66% and 79%, respectively.

Electrolysis
Four cases were run for hydrogen production via electrolysis. Central electrolysis for 2005 assumes a 125,000 kg/day wind electrolysis facility; grid electricity supplements the electricity from wind in the 2030 case (50/50 split between grid and wind) in order to increase the capacity factor of the electrolyzer from 41% in 2005 to 97% in 2030. Electrolyzer efficiency is 64% and 76% for the current and future cases, respectively. Typical efficiencies for today’s electrolysis systems are shown in Table 1.

| Table 1: Range of Energy Efficiencies for Today’s Electrolysis Systems |
|--------------------------|--------------------------|
| Alkaline HHV* Efficiency (%) | PEM HHV* Efficiency (%) |
| 57-75                     | 56-70                    |

*HHV is Higher Heating Value.

The cost of electricity is $0.049/kWh for wind in the 2005 case and $0.03/kWh for both grid and wind electricity in the future case. Hydrogen delivery is assumed to be by liquid hydrogen delivered by truck in the 2005 case and pipeline delivery in the 2015 and 2030 cases.

Distributed hydrogen production from wind was analyzed for 2005 and 2015. Electrolysis efficiencies are 64% and 76%, respectively. Capacity factors are 70% for each case with the grid/wind mix of 70%/30% for 2005 and 50/50 for the 2030 case. The cost of electricity is $0.052/kWh and $0.038/kWh for 2005 and 2030 cases, respectively.

The price of electricity is a major component of the estimated cost of hydrogen, as shown in Figure 5. The current and future required selling prices of hydrogen to obtain a 10% IRR at a central facility is $9.50 and $2.70/gge, respectively. Those for a distributed electrolysis pathway are $5.70 and $3.10/gge.

As shown in Figure 1, petroleum energy use for the four electrolysis cases is much lower than for gasoline internal combustion engine and hybrid vehicle cases. Figure 2 shows that greenhouse gas emissions are very low for the central wind electrolysis case. The petroleum energy use and resultant GHG emissions from distributed electrolysis are associated with hydrogen compression at the forecourt point of use, as well as the use of grid electricity. The energy efficiency for central electrolysis is 54% and 72% for the current and future cases, respectively. If produced at distributed locations, the energy efficiency increases to 61% and 73% for the current and future cases, respectively.
Biomass
We estimated the cost of centralized production of hydrogen from biomass for the 2005 and 2030 cases. The production system we analyzed includes major components including a gasifier and a reformer, high and low temperature water gas shift reformers, and a pressure swing adsorption unit. The biomass feedstock price is $38/bone dry ton for both cases. The assumed energy efficiency of the production unit is 45% and 52% for the current and future cases, respectively.

The petroleum energy use and carbon dioxide emissions for these cases stem from operations related to growing biomass and making it available to the hydrogen production process, as well as electricity use for production and hydrogen delivery. The required selling price of hydrogen to obtain a 10% IRR is $4.90 and $2.40/gge for the current and future cases, respectively.

Coal
We assessed centralized production of hydrogen from coal with sequestration of CO₂ for the 2005 and 2030 cases. The production system we analyzed includes major components including a coal gasifier and cleanup subsystem, high and low temperature water gas shift reformers, and a membrane separation unit. The coal feedstock price is $26.7/ton ($24.2/tonne). Plant capacity is 308,000 kg/day of hydrogen. Eight-five percent of the plant carbon dioxide is assumed to be captured and sequestered at a cost of $15 per metric tonne of carbon. The product hydrogen is separated at 300 psi and compressed before delivery to the hydrogen distribution system. Liquid hydrogen delivery is assumed for the current case; for the future case, delivery is as compressed gas by pipeline.

Total energy use is 5,100 and 3,200 Btu/mile for the current and future cases, respectively. Greenhouse gas emissions (210 and 60 g/mile) stem from the carbon dioxide that is not captured and sequestered, as well as from upstream energy use. The calculated required selling price of hydrogen to obtain a 10% IRR is $5.10 and $2.20/gge for the current and future cases, respectively. Pathway efficiencies for the two cases are 51% and 58%.

Nuclear
Thermochemical reaction cycles employ compounds that undergo reactions with water to produce hydrogen. The intermediate reaction products then undergo additional reactions to regenerate to the starting compounds before they are recycled to produce hydrogen again. Of the over 150 potential chemical reaction cycles that have been identified in the literature, a small set is being explored in conjunction with concentrated solar energy or nuclear energy to provide the requisite temperatures for the reaction cycles.

We analyzed one thermochemical reaction cycle, with nuclear energy providing the temperature at which the sulfur-iodine cycle reactions occur. Only a future case was examined because this technology is at an early stage of research and development. The nuclear fuel cost is $9.3/MWh; production process efficiency is 44%. The plant capacity is 768,000 kg/day. Delivery of hydrogen is in compressed state by pipeline.
The estimated well-to-wheels energy use and greenhouse gas emissions are 4,700 Btu/mile and 60 g/mile, respectively. The required selling price of hydrogen to obtain a 10% IRR is $3.20/kg; the pathway efficiency is predicted to be 42%.

**Biological Pathways**

**Photoelectrochemistry**

Photoelectrochemistry (PEC) can be employed to produce hydrogen in a one-step process in which water is split into hydrogen and oxygen directly upon illumination. PEC is in an early stage of research and development. Known light-absorbing semiconductor materials have either low efficiency (1%-2%) or low durability in an aqueous environment (tens of hours for materials with efficiencies approaching 10%). The U.S. DOE targets for 2015 are 10% solar-to-hydrogen conversion and 5,000 hours of durability. The goal for photoelectrochemical and biological processes is to develop these advanced technologies and verify the feasibility of these technologies to be competitive in the long term.5

Materials are needed that simultaneously possess sufficient band gap to capture and split photons efficiently, produce electrons-positive hole pairs at energy levels that drive electrochemical reactions to split water, and are durable in aqueous environments.

**Fermentation**

Several organisms can produce hydrogen via fermentation. The cost of feedstock and the molar yield of H₂ are two major barriers for fermentation technology. For example, a mole of glucose has sufficient energy to produce 12 moles of hydrogen, but known biological pathways only produce 2-4 moles, and most laboratories report yields of only 1-2 moles. The U.S. DOE’s 2015 program goal for dark bacterial fermentation is to realize a yield of six moles of hydrogen per mole of glucose and achieve six months of continuous production.

One approach to addressing the feedstock barrier is to screen and identify microbes capable of using cellulose and hemicellulose directly, in lieu of glucose, for H₂ production. This approach would provide a less expensive feedstock. An approach to improving molar yield is to perform genetic engineering by re-directing metabolic pathways preferentially toward H₂ production. Research is now underway to address these issues. Fermentative hydrogen production is accompanied by the co-production of organic acids (e.g. acetate, butyrate, propionate). These can be further processed by photosynthetic bacteria, which, in the light, are able to extract the remaining reductants from these molecules and to simultaneously produce hydrogen gas. When coupled to photosynthetic bacteria, fermentation has the potential to yield 12 moles of hydrogen per mole of glucose. Currently, the average reported light conversion efficiencies achieved by photosynthetic bacteria are around 1.9, and their carbon conversion efficiency is around 41% of the maximum. The U.S. DOE’s 2015 program goal is to realize a light conversion efficiency of 5% and a carbon conversion efficiency of 65% by the photosynthetic bacterial system, for a total period of production of about 1.5 months.5

**Photobiology**

Photobiological production of hydrogen is also in the early stage of research and development. It offers the promise of water splitting from solar energy in systems that do not require pure water and produce essentially no pollutants. Both eukaryotic green algae and prokaryotic cyanobacteria can produce hydrogen from water. These systems split water into oxygen reductants, and protons using photochemical processes, and hydrogenase enzymes recombine protons and reductants to produce hydrogen. In both the algae and cyanobacteria, the hydrogenases are sensitive to oxygen, which inhibits their production of hydrogen.

Research is underway on both types of biological systems to improve the efficiency of light capture, water splitting, and oxygen tolerance. The maximum light conversion efficiency that can be achieved by using photobiological systems is 10%-13%, under conditions where both hydrogen and oxygen are evolved simultaneously. An alternative photobiological method that results in production of pure hydrogen gas (without the need to generate an oxygen tolerant system) was developed under DOE’s funding a few years ago. This alternative method, which depends on the activation of a physiological switch that induces hydrogen photoproduction, has the potential to achieve maximum light conversion efficiencies of 1%. Currently, the second method has resulted in continuous hydrogen production of up to 6 months, at an estimated light conversion efficiency of 0.36% (at low light intensities).

The U.S. DOE’s 2015 target for algal hydrogen production efficiency is 5% with four hours of continuous production. The 2015 target for bacterial photoproduction is 4.5% with three months of continuous production.5
**Conclusion**

In this study we used the H2A and GREET models developed by the U.S. DOE to estimate hydrogen production costs and greenhouse gas emissions for a variety of fuels and production technologies. The following table shows hydrogen costs and pathway energy efficiencies for the technologies studied.

<table>
<thead>
<tr>
<th>Pathway</th>
<th>Required Hydrogen Selling Price (gge)</th>
<th>Required Hydrogen Selling Price (gge)</th>
<th>Energy Efficiency (Current Technology)</th>
<th>Energy Efficiency (Future Technology)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Natural Gas</td>
<td>$3.10</td>
<td>$2.00</td>
<td>66%</td>
<td>79%</td>
</tr>
<tr>
<td>Electrolysis (central)</td>
<td>$9.50</td>
<td>$2.70</td>
<td>54%</td>
<td>72%</td>
</tr>
<tr>
<td>Electrolysis (distributed)</td>
<td>$5.70</td>
<td>$3.10</td>
<td>61%</td>
<td>73%</td>
</tr>
<tr>
<td>Biomass</td>
<td>$4.90</td>
<td>$2.40</td>
<td>40%</td>
<td>49%</td>
</tr>
<tr>
<td>Coal</td>
<td>$5.10</td>
<td>$2.20</td>
<td>51%</td>
<td>58%</td>
</tr>
<tr>
<td>Nuclear</td>
<td>$3.20</td>
<td></td>
<td></td>
<td>42%</td>
</tr>
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**References**


